Title: FLAVANONE COMPOUND AND USES THEREOF Inventor(s): KUMAZAWA Serial No.: PCT/JP2004/008964

Docket No.: 50266-00001

David F. Dockery

(303) 338-0997

Fig. 1

Compound 1 - Physicochemical Properties

Appearance	white powder
Molecular formula	$C_{25}H_{28}O_{6}$
ESI-MS (m/z)	
Positive:	425.3 (M+H) ⁺
Negative:	423.5 (M−H) ⁻
UV $\lambda_{\max}^{\text{MeOH}}$ nm (ϵ)	288.5 (19,674)
IR (KBr) cm ⁻¹	3420, 2960, 2920, 1680, 1600, 1160
$[\alpha]_{0}^{24}$ (c 0.2, MeOH)	-5.8°
$[\alpha]_{D}^{25}$ (c 0.2, CHCl ₃)	+20.0°
MP	80~83°C
CD (MeOH) θ /deg	8470 (330), -46997 (290), 12833 (255)

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Fig. 2

NMR Data (Compound 1 in Acetone-da)

NMR Data (Compound 1 in Acetone-d ₆)				
Position	13	°C		'Н
2	77.21	СН	5.62	(1H, dd), J=2.9, 11.8 Hz
3 ,	43.26	CH ₂	2.66	(1H, dd), <i>J</i> =2.9, 17.2 Hz
			3.17	(1H, dd), <i>J</i> =11.8, 17.2 Hz
4	197.59	C .		
5	165.29	С	12.19	(-OH, s)
. 6	95.83	CH:	5.96	(1H, s)
·7	167.27	С		
8 .	96.79	СН	5.96	(1H, s)
9	164.65	C		
10	103.12	С		
1'	129.77	С		
2'	127,71	. C		
3'	144.08	С		
. 4'	145.56	С		
5'	113.49	СН	6.82	(1H, d), <i>J</i> =8.3 Hz
6'	118.55	СН	6.96	(1H, d), <i>J</i> =8.3 Hz
1"	25.15	CH ₂	3.55	(2H, d), J=6.3 Hz
2''	124.15	СН	5.18	(1H, t), J=6.3 Hz
3"	135.33	C		
4''	16.34	CH ₃	1.68	(3H, s)
5"	40.37	CH ₂	1.97	(2H, t), √=6.2 Hz
6"	27.34	CH ₂	2.05	(2H, m)
7"	125.02	СН	5.06	(1H, dt), J=1.9, 6.2 Hz
8"	131.74	С		
9"	25.75	CH ₃	1.60	(3H, s)
10"	17.68	CH ₃	1.55	(3H, s)

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Fig. 3

Compound 2 - Physicochemical Properties

Appearance	yellow powder
Molecular formula	$C_{25}H_{28}O_{6}$
ESI-MS (m/z)	
Positive:	425.0 (M+H) ⁺
Negative:	423.3 (M-H) ⁻
HRFAB-MS (m/z)	
calcd.:	425.1965(M+H) ⁺
found:	425.1968(M+H) ⁺
UV λ_{\max}^{MeOH} nm (ε)	288.0 (17.935)
IR (KBr) cm ⁻¹	3360, 2960, 2920, 1680, 1600
$[\alpha]_{\rm D}^{25}$ (c 0.2, MeOH)	-17.8°
MP	123∼126°C
CD (MeOH) θ /deg	11444 (332), -30028 (292), 7139 (254)

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Fig. 4

NMR Data (Compound 2 in Acetone-da)

	NMR Data (Compound 2 in Acetone-d ₆)				
Position	¹³ C			¹H	
. 2	80.13	СН	5.35	(1H, dd), <i>J</i> =2.9, 12.2 Hz	
3	43.54	CH ₂	2.74	(1H, dd), J=2.9, 17.1 Hz	
	·		3.12	(1H, dd), J=12.2, 17.1 Hz	
4	197.19	C			
5	165.24	С	12.17	(-OH, s)	
6	95.81	СН	5.95	(1H, s)	
7	167.28	С			
8	96.74	СН	5.95	(1H, s)	
9	164.31	C			
10	103.22	С			
1'	130.58	С			
2'	112.07	СН	6.91	(1H, d), <i>J</i> =2.2 Hz	
. 3'	145.26	С			
4'	144.30	С			
5'	129.02	С			
6'	119.97	сн	6.81	(1H, d), J=2.2 Hz	
1"	28.83	CH ₂	3.38	(2H, d), <i>J</i> =7.3 Hz	
2"	123.36	СН	5.38	(1H, m)	
3"	136.39	С .			
· 4"	16.21	CH ₃	1.73	(3H, s)	
5''	40.45	CH ₂	2.06	(2H. t), <i>J</i> =7.5 Hz	
6"	27.37	CH ₂	2.12	(2H, td), J=6.8, 7.5 Hz	
7''	125.07	СН	5.12	(1H, tq), $J=1.5$, 6.8 Hz	
8''	131.70	С		1.0, 0.0 112	
9''	25.80	СН₃	1.63	(3H, s)	
10"	17.71	CH ₃	1.57	(3H, s)	

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Fig. 5

Compound 3 - Physicochemical Properties

Appearance	yellow powder
Molecular formula	$C_{25H_{28}O_{6}}$
ESI-MS (m/z)	
Positive:	425.1 (M+H) ⁺
Negative:	423.2 (M-H)
UV λ_{\max}^{MoOH} nm (ϵ)	291.5 (16,833)
IR (KBr) cm ⁻¹	3380, 2960, 2920, 1680, 1600, 1450
$[\alpha]_{\rm D}^{\rm 23}$ (c 0.77, MeOH)	-3.94°
$[\alpha]_{\rm D}^{\rm 25}$ (c 0.2, CHCl ₃)	-6.5°
MP	172∼175°C
CD (MeOH) θ /deg	9773 (335), -26940 (293), 3399 (255)

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Fig. 6

		Compound	3 in Acetone-d ₆)
Position	13C		¹ H
2	79.85 CH	5.35	(1H, dd), J=3.0, 12.7 Hz
3	43.64 CH ₂	2.71	(1H, dd), J=3.0, 17.1 Hz
		3.12	(1H, dd), J=12.7, 17.1 Hz
4	197.26 C		
5	162.24 C	12.46	(-OH, s)
6	108.99 C		
7	164.76 C		
8	95.27 CH	6.03	(1H, s)
9	161.91 C	•	
10	103.09 C	i.	
1'	131.69 C		
2'	114.67 CH	7.03	(1H, s)
3'	145.95 C		
4'	146.28 C		
5'	115.97 CH	6.86	(1H, s)
6'	119.18 CH	6.86	(1H, s)
.1"	21.53 CH ₂	3.26	(2H, d), <i>J</i> =7.3 Hz
2"	123.44 CH	5.26	(1H, td), J=1.0, 7.3 Hz
3"	134.96 C		
4"	16.18 CH ₃	1.76	(3H, s)
5"	40.46 CH ₂	1.95	(2H, t), J=7.5 Hz
6"	27.38 CH ₂	2.05	(2H, m)
7"	125.12 CH	5.08	(1H, tt), J=1.0, 5.4 Hz
8"	131.54 C		
9"	25.77 CH ₃	1.62	(3H, s)
10"	17.66 CH ₃	1.56	(3H, s)

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Fig. 7

Compound 4 - Physicochemical Properties

Appearance	light brown gum		
Molecular formula	$C_{30}H_{36}O_{6}$		
FAB-MS (m/z)			
Positive:	493.3 (M+H) ⁺		
UV λ_{\max}^{MeOH} nm (ε)	292.0 (20,418)		
IR (KBr) cm ⁻¹	3400, 2960, 2920, 1640, 1600		
$[\alpha]_{\rm D}^{24}$ (c 0.2, MeOH)	+1.8°		
$[\alpha]_{0}^{25}$ (c 0.2, CHCl ₃)	+26.5°		
CD (MeOH) $ heta$ /deg	8810 (335), -30708 (293), 10510 (257)		

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Fig. 8

NMR Data (Compound 4 in Acetone-d₆)

	NMH	Data (C	ompound 4	4 in Acetone-d ₆)
Position	¹³ C			'н .
2	77.12	СН	5.59	(1H, dd), J=2.7, 13.5 Hz
3	43.49	CH ₂	2.65	(1H, dd), <i>J</i> =2.7, 17.2 Hz
			3.14	(1H, dd), J=13.5, 17.2 Hz
4	197.65	С		
5	162.27	С	12.47	(-OH, s)
6	108.96	C	,	
7 .	164.74	C ·		
8	95.29	CH	6.04	(1H, s)
9	162.27	C ,		
10	103.01	C .		
1'	129.96	С		
. 2'	127.59	С		
3,	144.04	С		·
4'	145.49	С	:	•
5'	113.50	СН	6.82	(1H. d), J=8.3 Hz
6'	118.51	CH .	6.96	(†H, d), J=8.3 Hz
1"	25.13	CH ₂	3.54	(2H, d), J=6.5 Hz
2"	124.15	- CH	5.18	(1H, t), J=6.5 Hz
3"	135.34	C		
4"	16.37	CH ₃	1.64	(3H, s)
. 5"	40.36	CH ₂	1.97	(2H, t), J=7.0 Hz
6''	27.35	CH ₂	2.04	(2H, m)
7"	125.02	СН	5.06	(1H, qt), J=1.2, 7.0 Hz
8"	-131.72	С		
9"	25.84	CH ³	1.69	(3H, s)
10"	17.67	CH ₃	1.55	(3H, s)
1′''	21.62	CH ₂	3.26	(2H, d), J=6.6 Hz
2'''	123.61	СН	5.24	(1H, gt), J=1.5, 6.6 Hz
3"'	131.17	С		
4'''	25.75	CH₃	1.61	(3H, s)
5'''	17.81	CH ₃	1.76	(3H, s)

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